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This research concerns sixteen projects of ten ICMA (Institute for Computational Mathematics and Applications) personnel, relating to the general area of computational fluid mechanics. Topics include the reduced basis method, flow through combustors, error estimation and singularities, dual variable transformations, differential equations on manifolds, energy stability, the conjugate gradient method and supercomputing calculations.

Short descriptions of these projects are included, along with references to published more complete presentations.

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Final Technical Report

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Period: 1 June 1984 through 31 May 1988

Title: Computational Fluid Dynamics

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A. ACCOMPLISHMENTS

The following is a brief summary of accomplishments under Grant AFOSR-84-0131. Reports and papers listed in Section B contain more detailed presentations and may be obtained from the investigators.

1. *The Reduced Basis Method for Algebraic Systems*

1.1 *Subspace-Projector Pairings.* Implementation of the reduced basis method requires the choice of a subspace and a projector onto that subspace. For an arbitrarily chosen subspace-projector pair, existence of the true solution curve is not sufficient to guarantee the existence of the corresponding reduced basis solution curve. However, when the former curve exists, it has been shown in [A1] that there are infinitely many subspace-projector pairings, each utilizing an *arbitrarily selected subspace*, under which the reduced basis solution curve exists. Moreover, the resulting error estimates are of the same nature as those that apply in the more familiar case when a subspace is paired with its orthogonal projector.

1.2 *Reduced Basis Additive Correction Methods.* Additive Correction Methods have been considered by a number of authors as a means of accelerating slowly converging iterative processes (see, for example, [A2]-[A4]). Furthermore, it has been recognized that additive correction is central to the basic idea of multigrid methods [A4-A5]. Although the reduced basis method in its original form appears to have little in common with additive correction, a class of such methods has been developed using the reduced basis concept [1]. Furthermore, it has been shown that in their "two-grid" form, certain multigrid methods are special cases of this class. The reduced basis point of view provides insight into the error reduction capability of such multigrid methods, and at the same time suggests additive correction variants that lie outside the scope of the usual multigrid formalism.

For example, an additive correction that is based on the span of translates of "presmoothed" iterates does not correspond to any usual "coarse grid" correction in the multigrid sense. However, it can be shown that if such corrections follow ν presmoothing iterations, and if the smoothing process is symmetrizable, then the result is at least as good as that which would have been obtained by doing ν iterations of the Chebyshev semi-iterative

method [A19] *with optimum parameters.* Furthermore, a model problem analysis shows that these corrections always incorporate the ability to remove completely *any* ν of the modes that remain in the presmoothed error. Details of these results will appear in [31].

2. *The Reduced Basis Method for Systems of Differential Equations*

Error Estimates for the reduced basis method solution of differential and differential-algebraic equation systems are contained in the Ph.D. thesis [2] by M.Y. Lin-Lee, under the direction of Professor Thomas Porsching. These estimates are local in the following two senses. First, they apply on a nontrivial, but possibly very small interval. Second, they require some point of the reduced curve to lie on the true solution curve. The recent research reported in [18] has removed the interval length restriction in the differential equation case and extended the error analysis to global versions of the methods in [2], thus effectively eliminating the second local aspect of that work. Furthermore, this work also incorporates the effects of the errors resulting from the numerical integration of the reduced basis ODE systems.

3. *Two-Fluid, Two-Phase Flow*

Additional theoretical results on the nature of the void fraction have been incorporated into [A6] resulting in the revision [3].

4. *Binary Gas Mixture Flow Through Combustors*

In an attempt to reduce the development cycle costs associated with design of gas turbine engine combustors, mathematical combustor models are being employed to provide information about performance trends and to predict velocity, pressure and thermodynamic property profiles in simulated practical combustion environments. It has been demonstrated that the dual variable method can be applied to the predictive model of the fluid dynamics associated with an axially symmetric centerbody combustor being studied at WPAFB. This work appeared in [4]. Modifications have been made to the industry standard program TEACH to allow for more efficient, local iteration. The same algorithm is also used in a dual variable version which shows even more

savings.

5. Error Estimation and Singularities

The central theme of this project concerns the errors arising in the computational solution of parameter-dependent equations of the form $F(z,\lambda) = 0$ where F is a given nonlinear mapping, z is the state variable representing the solution, and λ is a vector of parameters that characterize intrinsic properties of the system or extrinsic quantities influencing its behavior. In the case of fluid problems, the operator may be generated, for example, by the time-independent Navier Stokes equations together with the necessary boundary conditions.

In general, the solution set of such parametrized equations constitutes a differentiable manifold M of dimension equal to that of the parameter space Λ. While this fact is, of course, well known, we appear to have been the first who have been using this fact as the basis for a consistent study of the numerical problems for these equations. Our results have begun to show clearly the value and power of this geometric approach.

The basic procedures for the computational analysis of such a manifold M are the continuation methods. When M has dimension $p > 1$, these methods require a restriction to some path on M and then produce a sequence of points along that path. Obviously, it is not easy to develop a good picture of a multi-dimensional manifold solely from information along such paths. This led us recently to the development of methods for the computation of simplicial approximations of p-dimensional subsets of M (see [25], [26]). Besides these methods for computing specific sets of points on M, another important class of numerical procedures concerns the detection and computation of foldpoints on M with respect to a given coordinate space T, such as the natural parameter space Λ, (see [5], [7], [19], [21]).

For numerical considerations, an important aspect of this theory concerns the estimation of the various errors arising in the computations. These errors fall into several classes. First of all, there is the important question of the discretization errors which in this setting turns out to be the "distance" between the manifolds defined by a given differential equation and by its discretization, respectively. This has been the topic of a series of papers by J. P. Fink and W. C. Rheinboldt with partial support under this grant. See the earlier articles [A7], [A8] and then [6] and [16]. In particular, in the last named paper [16] we have been the first to analyze the case

of multi-dimensional manifolds which is of increasing importance in applications.

An essential aspect of these discretization studies concerns the question as to the exact definition of the error between a solution manifold and its approximation. Obviously, the error depends on which points are to be compared. In the cited papers it was shown that this correspondence between the points on the two manifolds has to be defined by appropriate local coordinate systems. In other words, the resulting error is controlled by the choice of the local coordinate system, and, since the error measure must be physically meaningful, not all local coordinate systems are equally desirable. This question becomes particularly acute in the vicinity of singular points where the behavior of the solutions may be subject to change.

This connection between the choice of the local coordinate systems and the singularity behavior of a point has led us to a closer study of admissible coordinate systems at foldpoints. But the results in [5] and [7] also suggest that the open questions about the proper choice of the coordinate system for physically meaningful error measures requires a much closer look at the characterization of foldpoints on manifolds and at the methods for their computation.

Besides the discretization errors there are various other computational errors which arise in the analysis of the solution manifolds of parametrized equations. In particular, both in the continuation methods and in the simplicial approximation methods, mentioned above, we encounter the following sources of errors:

(a) Errors associated with the predictor and corrector:

(a1) Estimation of the prediction error

(a2) Control of the termination error

(a3) Control of the effect of round-off

(b) Errors associated with the choice of local coordinate system:

(b1) Estimation of the domain of validity of this coordinate system,

(b2) Control of the range of applicability of the moving frame algorithm in the simplicial

approximation method.

In connection with foldpoints computations, various further error questions arise; they will be discussed in the next subsection. During the past year a study of these and related error questions has begun and will be continuing during the next year.

6. *Detection and Computation of Singularities*

As noted in the previous subsection, the solution set of a parametrized equation $F(z, \lambda) = 0$ represents, in general, a differentiable manifold in the combined space of the state variable and the parameter vector. This requires a regularity assumption which is not very restrictive in applications, but which -- from the viewpoint of singularity theory -- implies the use of a suitable "unfolding". In most practical problems a host of very natural unfoldings suggest themselves. However, the particular choice of unfolding affects the location and type of the resulting foldpoints on the manifold and with it also the error questions raised in the previous subsection.

Our previous work in this area concentrated on a study of the differential geometric aspects of the problem. In the already mentioned papers [5], [7] we used the tangent map to develop a geometrically instructive and coordinate free treatment of foldpoints. Then in [21] is was shown that it is possible to reformulate in this setting some of the basic results of bifurcation theory related to computational aspects. In particular, the bifurcation sets appear as certain cuts of the solution manifold. This in turn corresponds to the consideration of particular augmented equations and hence opens up a new approach to the study of effective augmentations for the computation of singular points. Such a study was begun in [19].

On the basis of the results in [21] R. X. Dai, a Ph.D. student at the University of Pittsburgh under the direction of Professor Rheinboldt, has been working on a new method for specific class of foldpoint problems. More specifically, a new minimal augmentation of the original equations have been devised for the computation of so-called (p,1,1) foldpoints. For the resulting systems an efficient local corrector process has been developed which allows for the continuation along a path of such foldpoints. In addition the approach does appear to open up the possibility of extending the simplicial approximation approach mentioned in the previous subsection to sub-manifolds of (p,1,1) foldpoints. This is currently being studied. The techniques have already been applied to a variety of test problems with excellent success. A comprehensive report will be forthcoming within a few

months.

As noted in the previous subsection, there are numerous error questions, we have investigated, arising in the different processes for computing foldpoints on a solution manifold. We mention here only the principal topics:

(a) Detect a foldpoint in a neighborhood of a given set $x^1, \ldots, x^k$ of points.

(b) For a given approximation x of a foldpoint x* of the manifold estimate the distance $||x-x^*||$ between these points.

(c) For foldpoints of a specific type develop iterative processes which are locally convergent to these points from any sufficiently close approximation.

(d) If x_h is a computed foldpoint of the discretized equations which approximates a foldpoint x of the original differential equations, compute an estimate of the distance $||x - x_h||$.

7. *Finite Element Formulation of the Streamfunction-Vorticity* Equations

The Navier-Stokes equations can be written in primitive variable formulation, in terms of the streamfunction as a fourth order problem or as two second order equations in the streamfunction-vorticity formulation. In the linear case the fourth order problem for the streamfunction is the well-known biharmonic equation. Although the primitive variable formulation has received the most attention, the streamfunction-vorticity formulation is also of considerable interest in two dimensional domains. That is partly due to the fact that only two, as opposed to three, fields are to be computed; but it is mainly due to the fact that the incompressibility constraint is avoided through the introduction of the streamfunction.

Several theoretical and practical issues arising in the finite element approximation of the streamfunction-vorticity equations have been studied. Initially error estimates for the linear problem were investigated. Since the velocity is expressed in terms of the derivatives of the streamfunction, it is of practical concern to ascertain if these derivatives are optimally approximated for choices of elements. Previous analyses concerning this problem were improved upon and the optimality of the error verified in [A10].

Other issues arising in the finite element approximation of the streamfunction and vorticity include computations in multiply connected domains, the use of low order elements, the incorporation of a variety of boundary conditions into the weak formulation, estimates for the errors in the finite approximations for the nonlinear problem and the recovery of the primitive variables. A preliminary report on computations in multiply connected domains using low continuity finite element spaces was presented in [11]. A comprehensive report dealing with all of the theoretical and practical issues mentioned above as well as presenting numerical examples is given in [12].

8. *A Finite Element Analysis of MHD Flow*

The equations governing the steady flow of incompressible electrically conducting fluids in the presence of a given magnetic field can be expressed as

$$-\frac{1}{n^2}\Delta \underline{u} + \frac{1}{N}(\underline{u}\cdot\nabla\,\underline{u}) + \nabla\phi - (\underline{B}\times\nabla\phi) - (\underline{u}\times\underline{B}\times\underline{B}) = 0$$

$$-\Delta\phi + div\,(\underline{u}\times\underline{B}) = 0$$

$$div\ \underline{u} \quad = 0$$

where $\underline{u}$ is the velocity, p the pressure, ϕ the electric potential, $\underline{B}$ the magnetic field and N, n given dimensionless parameters. By rewriting certain terms using vector identities and using appropriate spaces, one can obtain a weak formulation for this problem that is similar to one for the Navier-Stokes equations written in terms of primitive variables (see [A11]). The purpose of using such a weak formulation is to take advantage of the results already proved in [A11]. Specifically, the weak formulation is to find $\underline{u} = (\underline{u},\phi) \in \underline{W}$, $p \in L_o^2$ such that

$$a(\underline{u},\underline{v}) + a_1(\underline{u},\underline{u},\underline{v}) + b(\underline{v},p) = (f,\underline{v}) \quad \text{for } all \quad \underline{v} \in \underline{W}$$

$$b(\underline{u},\chi) = 0 \qquad \text{for } all \quad \chi \in L_o^2$$

where

$$a(\underline{u},\underline{v}) \quad = \frac{1}{n^2}\int \nabla\underline{u}:\nabla\underline{v} + \int \{\nabla\phi-(\underline{u}\times\underline{B})\}\cdot\{\nabla\psi-(\underline{v}\times\underline{B})\}$$

$$a_1(\underline{u}, \underline{u}, \underline{v}) = \frac{1}{2N} \int \{\underline{u}\cdot\nabla\, \underline{u}\cdot\underline{v} - \underline{u}\cdot\nabla\, v\cdot u\}$$

$$b(\underline{v}, \chi) \quad = -\int \chi\, div\ \underline{v}$$

and $\underline{W} = \underline{H}_o^1 \times H_o^1$, $L_o^2 = \{\phi \in L^2 : \int_\Omega \phi = 0\}$.

The continuity and stability conditions necessary to guarantee existence and uniqueness of the solution of the weak problem have been proved. In addition, an error estimate for the finite element approximation of the weak problem has been obtained. These results, as well as a discussion of an iterative method for solving the discrete problem will be presented in [13].

9. *Dual Variable Transformations*

The dual variable method, originally developed in the context of finite difference discretizations of transient incompressible Navier-Stokes equations [A9], is a technique to considerably reduce the size of the linear system to be solved at each time step. The method involves

(1) the determination of the rank of the discrete divergence operator, A,
(2) the determination of a basis for the null space of A, and
(3) the calculation of a particular solution of the discrete continuity equation.

In [8] a finite element implementation of the dual variable method is presented using quadrilateral piecewise bilinear velocity/constant pressure elements. Algorithms for the determination of a basis for the null space of the discrete divergence operator and a particular solution are presented.

In [9] a finite difference discretization of the Navier-Stokes equations describing a compressible flow problem is viewed as a system defining flows on an associated network. This observation then provides a means of applying the dual variable method to economize on their numerical solution.

The nature of the aerodynamics in and around such structures as cavities and deflectors or spoilers on various aircraft configurations was investigated using the dual variable method [10].

A summary of the dual variable method is given in [14].

Iterative methods are under investigation for the solution of the linearized finite difference discretizations involved in the dual variable method. The generic form of dual variable system suggests a splitting in which a Stieltjes matrix is to be solved at each step. The method has been implemented for two dimensional domains and convergence properties were investigated as part of a Ph.D. thesis by George Mesina [35], under the direction of Professor Charles Hall.

10. *Fluid Flow on Curved Domains*

A finite difference scheme was derived for two-dimensional, transient, incompressible Navier-Stokes problems in which the flow domain Ω is a bounded simply-connected region for which there exists a C^2 invertible mapping τ onto the unit square:

$$\tau : \Omega \rightarrow S \equiv [0,1]\times[0,1]$$

The *transformed* Navier-Stokes problem is

$$div\ \underline{\Phi} \equiv \Phi_{i,r_i} = 0$$

$$v_{i,t} + \frac{\Phi_j}{|J|} v_{i,r_j} = -p_{r_j} r_{j,x_i} + \frac{\mu}{|J|} (\beta_{jk} v_{k,r_k})_{r_j} + f_i \quad i = 1,2$$

subject to initial condition

$$\underline{v}(\underline{r}, 0) = \underline{a}(\underline{x}(\underline{r})) \ , \underline{r} \in S$$

and boundary condition

$$\underline{v}(\underline{r}, t) = \underline{0} \ , \underline{r} \in \partial S \text{ and } t > 0 \ ,$$

where, $\underline{v}(\underline{r}, t)$ is velocity, p is pressure, the Jacobian matrix

$$J = [x_{i,r_j}],$$

$$[\beta_{ij}] = |J| J^{-1} (J^{-1})^T$$

$$\underline{\Phi} = |J| J^{-1} \underline{v} \ .$$

The finite difference discretization of the above equations is proven to be unconditionally stable and convergent. They also reduce to the well known Krzhivitski and Ladyzhenskaya scheme [A12] for rectangular domains, e.g., τ the identity. This work was the subject of a Ph.D. Dissertation of John Ellison, under the direction of Professors Charles Hall and Thomas Porsching [A13] and appeared in [17].

11. *Differential Equations on Manifolds*

As noted earlier, equilibrium problems arise naturally in continuum and fluid mechanics as a set of nonlinear equations of the form

$$F(\underline{z}, \underline{\lambda}) = 0 \tag{1}$$

where $\underline{z}$ is from the state space Z and $\underline{\lambda}$ is from a p dimensional parameter space. Then the equilibrium manifold is the set of solutions to (1) in $D \subset X = Z \times \Lambda$; that is

$$M = \{(\underline{z}, \underline{\lambda}) \in D \mid F(\underline{z}, \underline{\lambda}) = 0\} \tag{2}$$

The parameters $\underline{\lambda}$ and states $\underline{z}$ may be required to satisfy a differential equation of the form

$$A(\underline{x})\dot{\underline{x}} = \underline{G}(\underline{x}) \tag{3}$$

where $\underline{x} = (\underline{z}, \underline{\lambda})$. We then interpret (3) as a *differential equation on the manifold* (2), DEM for short. Equations (1) and (3) together,

$$\begin{cases} F(\underline{x}) = 0 \\ A(\underline{x})\dot{\underline{x}} = \underline{G}(\underline{x}) \end{cases}$$

form what is called a *differential-algebraic equation* (DAE).

Two applications of interest to the investigators in which DEM's occur are:

(i) *Incompressible Fluid Flow.* The continuity equation is an algebraic constraint of the form (1) and the time-dependent Navier-Stokes equations are the differential equation.

(ii) *Punch Stretching of Sheet Metal.* The principle of virtual work provides a force equilibrium equation which defines an equilibrium manifold upon which one seeks solutions to differential constitutive laws of the form (3).

In [20], a new numerical method was presented for computer simulations of punch stretching of sheet metal. Most current approaches to finite element modeling of large deformation, elastic-plastic sheet metal forming use a rate form of the equilibrium equations and then must correct at each time step to insure that equilibrium is satisfied. Such methods are referred to as *incremental methods*. The new method, a *DEM* approach discretizes the more fundamental equilibrium equations in non-rate form and insures equilibrium of forces at each time step. Formulating the problem as a DEM or DAE also allowed for solution of the discretized system using off-the-shelf software such as LSODI. Numerical experimentation indicated that the DEM approach was computationally much more efficient than the incremental approach.

12. *Energy Stability of Viscous Incompressible Flows*

The problem of determining sufficient conditions for the flow of a viscous incompressible fluid to be stable under arbitrary disturbances was examined. This problem is of importance in the study of turbulence and the transition which occupies a region of space and is subject to a prescribed velocity distribution on the boundary, will alter radically or only slightly in nature if it is perturbed at some instant.

The question of stability can be addressed by either standard linear perturbation techniques or by the energy method; the latter is chosen in this work. Although the great majority of stability calculations use linear stability analysis, the method has the drawback that it allows only perturbations which are infinitesimal in magnitude. This rules out perturbations of finite size and hence cannot give accurate information in many cases. The energy method allows arbitrary disturbances but its shortcoming is that the disturbances do not necessarily satisfy the Navier-Stokes equations, and thus the stability criterion will be more restrictive than in the actual physical situation. However, the energy stability analysis is based on the Navier-Stokes equations and is nonlinear in nature due to the fact that no linearizations of the equations are done. The method is mathematically rigorous and does give insight into the physical situation.

The question of energy stability of a flow can be formulated as a linear generalized partial differential eigenvalue problem even though the analysis is based on the nonlinear Navier-Stokes equations. Essentially, the procedure is to obtain an equation for dK/dt where K is the kinetic energy of the disturbance, μ, and then to determine conditions which guarantee that the kinetic energy tends to zero as time increases. A standard

eigenvalue problem is used, where stability is governed by the dominant eigenvalue. Specifically, we have that the flow is stable for Reynolds number less than $1/\lambda$ where λ is the dominant eigenvalue of the problem

$$\begin{aligned} \Delta \underline{u} - \mathit{grad}\, \phi &= \lambda\, \underline{u} \cdot D \\ \mathit{div}\, \underline{u} &= 0\,, \\ \underline{u} &= 0\ \mathit{on\ the\ boundary}\ . \end{aligned} \tag{1}$$

Here D is the deformation tensor of the unperturbed flow.

A finite element method is used to approximate the dominant eigenvalue of (1). In particular, the weak form considered is to find nonzero $\underline{u} \in \underline{H}_o^1$, $\phi \in L^2$ and $\lambda \in R$ such that

$$\begin{aligned} \int \nabla \underline{u} : \nabla \underline{v} + \int \phi\, \mathit{div}\, \underline{v} &= \lambda \int \underline{u} \cdot D \cdot \underline{v} \quad \text{for all } \underline{v} \in \underline{H}_o^1 \\ \int \chi\, \mathit{div}\, \underline{u} &= 0 \qquad \text{for all } \chi \in L^2 \end{aligned} \tag{2}$$

where L^2 is the space of all functions which are square integrable and $\underline{H}^1$, $\underline{H}_o^1$ denote the usual Sobolev spaces. To approximate the solution to the weak problem (2), finite dimensional subspaces $\underline{V}^h \subset \underline{H}_o^1$ and $W^h \subset L^2$ are chosen which depend upon a parameter $0<h<1$ tending to zero. The approximate problem is defined analogous to (2) where the solution is sought in the finite dimensional subspaces. Once bases for $\underline{V}^h$ and W^h are chosen, the approximate problem is equivalent to an algebraic generalized eigenvalue problem. An estimate for the error in λ and its Galerkin approximation is given in [A14].

As proposed, a code was developed which uses a mixed finite element method for approximating the dominant eigenvalue of (1). The program was used to determine a range of Reynolds numbers for which the flow is guaranteed to be stable for the examples of plane shear flow and Poiseuille flow.

The first example is the simple case of flow in a channel of width $0<y<d$ where the initial velocity is given by the vector $(ky,0)$, the deformation tensor is given by $D_{ij} = 0$ for $i = j$ and $D_{ij} = .5k$ for $i \neq j$, $i,j = 1,2$ and the Reynolds number is kd^2/λ. The channel is assumed infinite in length. The computed Reynolds number for a channel of length L is given below.

1/L	1	1/2	1/3	1/4	1/5

Re No.	289.87	201.42	186.975	182.11	180.01

Using the above calculations the extrapolated value at $1/L = 0$ is 177.4 which is in good agreement with the value of 177 published by Orr.

The second problem of determining the stability of Poiseuille flow in a pipe is of more interest physically and has been studied by many authors. For this example the formulation (1) makes sense in an unbounded domain when the solutions are single-valued in θ and periodic in z. To this end, the solution is assumed of the form $\underline{u}(r, \theta, z) = \underline{U}(r, \alpha, \beta)\, e^{i(\alpha z + \beta\theta)}$ where β is an integer. This form is substituted into (1) and the following system results

$$Lu - i\left[\frac{2\beta}{r^2}\, v\right] - \phi_r = -\lambda r w$$

$$Lv + i(2\beta/r^2\, u - \beta/r\, \phi) = 0$$

$$\hat{L}w - i\alpha\phi = -\lambda r u$$

$$\frac{1}{r}\,\frac{\partial}{\partial r}\,(ru) + i\left[\frac{\beta}{r}\, v + \alpha w\right] = 0$$

$$u, v, w \text{ bounded at } r = 0$$

$$u = v = w = 0 \text{ at } r = 1$$

where $\underline{U} = (u, v, w)$, $Lu = \frac{1}{r}\,\frac{\partial}{\partial r}\,(ru) - \left[\frac{\beta^2+1}{r^2} + \alpha^2\right]u$, $\hat{L}u = Lu + u/r^2$.

Note that these equations form a complex one-point boundary value problem with a singularity at the origin. The weak formulation must incorporate an appropriate boundary condition for the velocity at $r = 0$. The particular weak from considered is the following: Find $u, v, w \in H_1$, $\phi \in H_2$, $\lambda \in R$ such that for all $\xi \in H_1$, $\chi \in H_2$,

$$
\begin{cases}
\int u_r \xi_r r\,dr + \int C_1 \frac{u}{r}\xi dr + i\int \frac{Z\beta}{r} v\xi dr - \int \phi \frac{\partial}{\partial r}(r\xi)dr = \lambda \int w\xi r^2 dr \\
\int v_r \xi_r r dr + \int C_1 \frac{v}{r}\xi dr - i\int \frac{2\beta}{4} u\xi dr + i\int \beta\phi\xi dr = 0 \\
\int w_r \xi_r r dr + \int C_2 \frac{w}{r}\xi dr + i\alpha\int \phi\xi r dr = \lambda \int u\xi r^2 dr \\
-\int \frac{\partial}{\partial r}(ru)\chi dr - i\int \beta v\chi dr - i\int \alpha w\chi r dr = 0 \\
\text{where } C_1 = \beta^2 + 1 + \alpha^2 r^2,\ C_2 = C_1 - 1
\end{cases}
$$

for appropriate spaces H_1 and H_2.

With this weak formulation the condition imposed on the velocity at $r = 0$ is $ru_r = rv_r = rw_r = 0$, which is a natural boundary condition. This problem was discretized using piecewise linear elements. The results obtained agree with those of Joseph and Carmi [A15]. However, their numerical calculations were unnecessarily complicated. For example, different techniques for the various cases such as $\alpha = 0$ and $\alpha \neq 0$ had to be employed as well as using Frobenius series as starting values near the origin. Specifically, the value of 81.5 was obtained as a sure limit of stability and corresponded to the case $\alpha = 1$, $\beta = 1$. This agreed with Joseph and Carmi's result and confirmed the fact that the value of $R = 180$, which was previously believed to be a sure limit of stability, is incorrect. This work is discussed in a paper in preparation [23].

13. *The Conjugate Gradient Method on Supercomputers.*

The application of the preconditioned conjugate gradient (PCCG) method to the solution of the large, sparse linear systems resulting from the discretization of partial differential equations on regular and irregular domains was investigated. The primary goal was the efficient implementation of the PCCG method on vector supercomputers. In [24], this goal was met by the introduction of

(i) A data structure which is suitable for manipulation on vector machines,

(ii) Preconditioned matrices which are effective for general sparse matrices, and

(iii) Numbering schemes for both regular and irregular grids, which are amenable to adequate vectorizations.

14. *The Numerical Solution of Transport Problems*

The question of finding schemes for approximating the solution of transport problems ($\varepsilon = 0$) and diffusive transport problems ($0 < \varepsilon \ll 0(1)$) is a central problem in computational fluid dynamics and combustion

theory. Frequently, efficient schemes are required which have high accuracy, preserve positivity, minimize dispersive effects, minimize grid orientation effects, etc.

An additive correction algorithm proposed in [A17] was considered for the 1-D equilibrium problem:

$$\begin{cases} -\varepsilon u'' + f(x)u' + g(x)u = g(x) \,, \; 0 < x < 1 \\ u(0) = \alpha \,, \; u(1) = \beta \,. \end{cases} \tag{1}$$

An exact analysis of the deferred correction algorithm was performed in [27], accounting for layer effects, via the theory of discrete barrier functions. This analysis established that in outer layer regions (regions of fixed distance $\delta > 0$ from layers) the scheme converges uniformly in ε with accuracy given by the high accuracy "defect" operator. The influence of discrete layer terms was clarified in [27] also. A mesh refinement process is naturally suggested by this analysis, which also gives a bound upon the region of assured $0(h^2)$ accuracy.

Next the case of 2-D equilibrium transport ($\varepsilon = 0$) and diffusive transport ($\varepsilon > 0$) problems was considered $u = u(x, y)$ satisfies

$$\begin{cases} -\varepsilon \Delta u + v_1 u_x + v_2 u_y + gu = q \,, \; in \; \Omega \subset R^2 \,, \\ u = \alpha \; on \; \partial\Omega \,, \; 0 \le \varepsilon \ll 0(1) \,. \end{cases} \tag{2}$$

We have focused our attention on methods which strictly preserve positivity. [A 2-D filtering technique which approximately preserves positivity in the deferred correction methods previously discussed was introduced in [A18]]. The simplest way to satisfy this requirement is with difference stencils which are of positive type.

In [28] the spurious diffusive effects of positive type schemes were investigated for (2). Specifically, the presence of anisotropic crosswind diffusion was studied. It was shown in [28] that, except when the transport direction is precisely aligned with the mesh, there does not exist a positive type scheme with zero spurious crosswind diffusion. The precise amount of this diffusive term is given in [28]. In [32], this analysis was taken one step further. The principal axes of diffusion for difference schemes were defined. By comparing these to the physical flow, a general methodology for comparing difference schemes and parameter selection in a given scheme is obtained.

In parallel, a much more ambitious approach to 2-D transport problems has been investigated. Monotone (i.e. inverse positive) type schemes for transport, transport-diffusion and transport-diffusion-reaction equations have been studied. Monotone schemes can, in principle, overcome many of the inherent barriers in positive type

methods. However, the inherent global and nonlinear character in generating monotone stencils presents a severe challenge.

Recently, there have been three breakthroughs at ICMA on this question. The first is that a methodology has been developed for reducing to sequential linear systems these global nonlinear consistency conditions. Thus, a technique has been developed for generating a class of novel monotone type difference schemes for general boundary value problems. This class contains a number of free parameters which can be used to enforce other desirable features e.g., high accuracy, minimal dispersive or diffusive properties, etc.

Secondly, a "collage" type theorem for monotone and positive type matrices has been proven. General monotone (inverse positive) matrices lack the algebraic structure of matrices of positive type. Thus, it is necessary to give a systematic procedure for combining monotone type stencils with other stencils to preserve stability in complex convection-diffusion-reaction problems. This collage theorem is a major step to developing a general theory which will specify the correct procedures.

These breakthroughs are a very general approach/methodology for deriving schemes with assured stability and assured preservation of positivity. To complete the picture, we are currently working on generating large classes of novel schemes for 2-D transport problems and analysis of the error the schemes generated. These would then be applied to many specific problems including combustion and fluid flow.

15. *Problems with Memory in Mathematical Physics*

Progress has been made in a tangentially related area of applied mathematics: physical processes incorporating delay on memory effects. For problems with (possibly infinite) delay:

$$\begin{cases} \dot{x}(t) + \int_{R^+} g(t, s, x(t), x(t-s))d\mu(s) = f(t), t \in R^+, \\ x(s) = \phi(s) \quad , \quad s \in R^-, \end{cases} \tag{1}$$

a global existence theory has been developed in [29] where the asymptotic behavior of solutions is also considered. In a companion paper [30], general conditions upon g and μ are given which ensure exponential asymptotic stability of the initial value problem. Thus, [29], [30] give a fairly complete picture of the behavior of solutions to (1) under a very mild nonresonance type condition upon g.

16. *3-D Fluid Flow Calculations on the CRAY XMP-48*

There is a rather large (6400 flow cell) version of the 2-D fluids code ALGAE [10] which typically takes overnight on a VAX 8650 to get one time-step finished. We needed such a large version in a fluids simulation of aircraft cavity flows, and found that we could get 300 time steps (often needed to get a steady state) finished on a CRAY XMP-48 within a 24 hour period. However, we noticed that this code was extremely slow and that 75-90% of the CPU time on the CRAY was being used by the solver. One obvious conclusion was that any practical 3-D code would have to be developed in a supercomputing environment using very efficient vectorized solvers.

Because of a short term need to make the CRAY XMP-48 version of ALGAE more efficient, and to give us some experience with high efficiency solvers of linear systems on the CRAY, we attempted to unravel the bookeeping in ALGAE to produce the final equations in matrix-vector form without turning on ALGAE's inefficient (on the CRAY) frontal solver. This latter feature, combined with ALGAE's link-list bookeeping, provides its excellent capability for efficient solution of a complicated geometry on computers with limited storage. However, on a large-memory machine devoted to vector efficiency and with parallel capability, the frontal solution can be hard to vectorize, and link-list bookeeping requires re-organization in vector form to get reasonable efficiency on a supercomputer such as the XMP-48. We had hoped to modify ALGAE to simply generate the matrices without turning on the frontal solver so we could call one of the high efficiency solver packages on the CRAY.

This turned out to be a coding nightmare, so it was decided to move on to a new coding for the 3-D version. We have extended the dual variable method [A9] to incompressible flow in three dimensions and a graduate student, Ms. Ye, under the direction of Professor Charles Hall has developed an algorithm for the construction of "countries" or faces of the associated network. A node-oriented system has been planned on domains that are imbedded in rectangular parallelopipeds.

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